



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:01 PM BST

PDB ID : 3JAT
EMDB ID: : EMD-6352
Title : Cryo-EM structure of GMPCPP-microtubule (14 protofilaments) decorated with kinesin
Authors : Zhang, R.; Nogales, E.
Deposited on : 2015-06-20
Resolution : 3.50 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

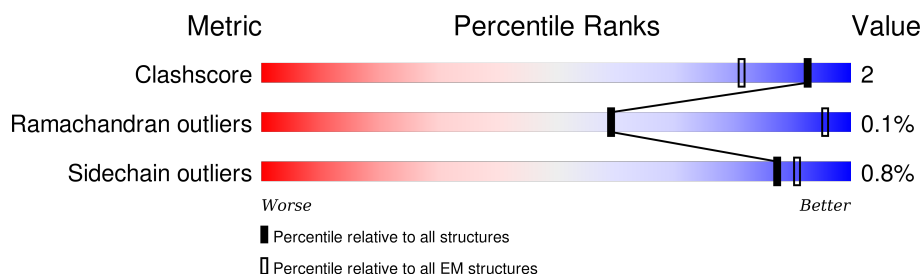
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	451	90% 5%
1	C	451	90% 5%
1	E	451	91% 5%
1	J	451	92% 5%
1	K	451	91% 5%
1	L	451	91% 5%
2	B	445	89% 7% .
2	D	445	90% 6% .
2	F	445	90% 6% .

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Mol	Chain	Length	Quality of chain
2	G	445	<div><div></div><div>90%</div><div>5%</div><div></div></div>
2	H	445	<div><div></div><div>90%</div><div>6%</div><div></div></div>
2	I	445	<div><div></div><div>91%</div><div>5%</div><div></div></div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 40500 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

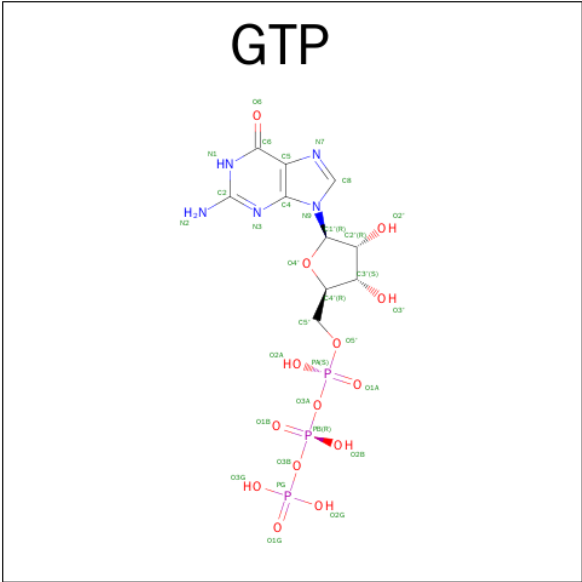
- Molecule 1 is a protein called Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	428	Total	C	N	O	S	0	0
			3342	2122	571	628	21		
1	J	428	Total	C	N	O	S	0	0
			3342	2122	571	628	21		
1	C	428	Total	C	N	O	S	0	0
			3342	2122	571	628	21		
1	L	428	Total	C	N	O	S	0	0
			3342	2122	571	628	21		
1	A	428	Total	C	N	O	S	0	0
			3342	2122	571	628	21		
1	K	428	Total	C	N	O	S	0	0
			3342	2122	571	628	21		

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	426	Total	C	N	O	S	0	0
			3342	2101	572	644	25		
2	G	426	Total	C	N	O	S	0	0
			3342	2101	572	644	25		
2	D	426	Total	C	N	O	S	0	0
			3342	2101	572	644	25		
2	I	426	Total	C	N	O	S	0	0
			3342	2101	572	644	25		
2	B	426	Total	C	N	O	S	0	0
			3342	2101	572	644	25		
2	H	426	Total	C	N	O	S	0	0
			3342	2101	572	644	25		

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
3	E	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	J	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	C	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	L	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	A	1	Total	C	N	O	P	0
			32	10	5	14	3	
3	K	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
4	G	1	Total	Mg	0
			1	1	
4	J	1	Total	Mg	0
			1	1	
4	D	1	Total	Mg	0
			1	1	
4	K	1	Total	Mg	0
			1	1	
4	E	1	Total	Mg	0
			1	1	
4	H	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total 1	Mg 1	0
4	I	1	Total 1	Mg 1	0
4	C	1	Total 1	Mg 1	0
4	A	1	Total 1	Mg 1	0
4	L	1	Total 1	Mg 1	0
4	F	1	Total 1	Mg 1	0

- # G2P

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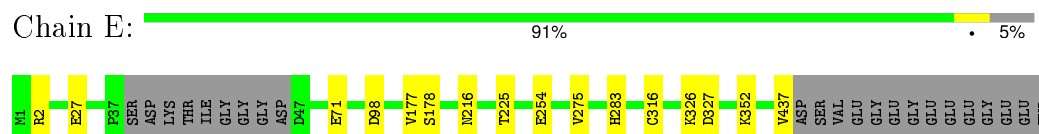
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
5	H	1	32	11	5	13	3	0

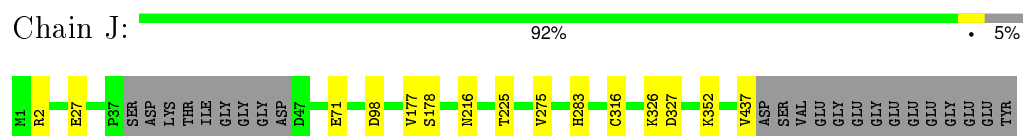
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

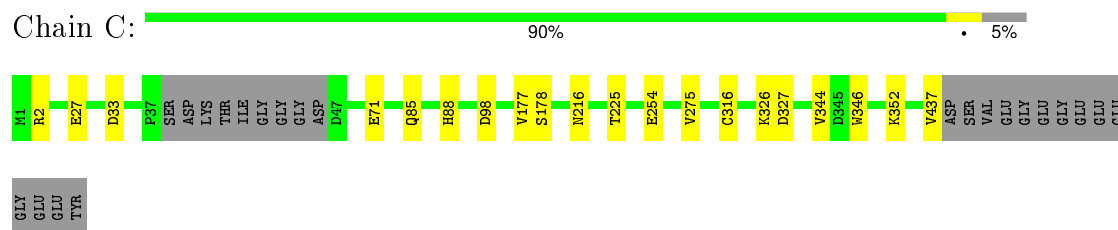
- Molecule 1: Tubulin alpha-1B chain



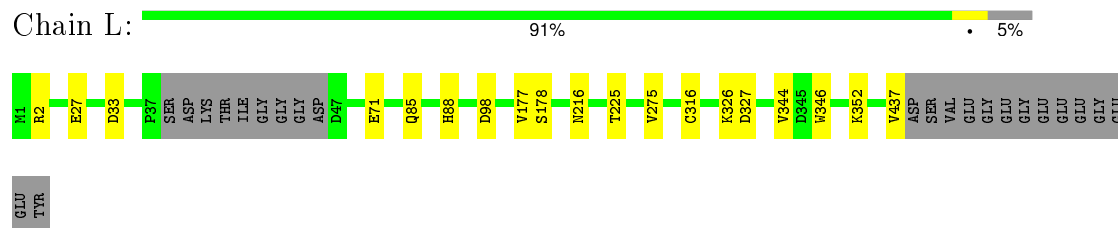
- Molecule 1: Tubulin alpha-1B chain



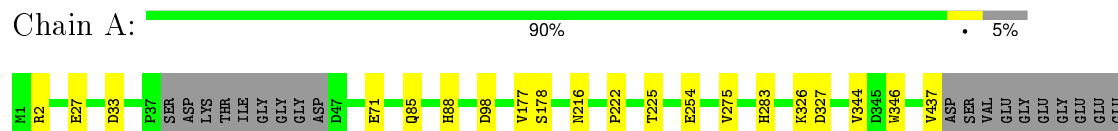
- Molecule 1: Tubulin alpha-1B chain



- Molecule 1: Tubulin alpha-1B chain



- Molecule 1: Tubulin alpha-1B chain



GLY
GLU
GLU
TYR


- Molecule 1: Tubulin alpha-1B chain

Chain K:  91% 5%

M1 R2 E27 P37 SER ASP LYS THR ILE GLY GLY ASP D47 E71 H88 D98 V177 S178 N216 T225 V275 H283 C316 K326 D327 V344 D345 W346 K352 W407 V437 ASP SER VAL GLY GLY GLY GLU GLU GLU GLU

GLU
TYR


- Molecule 2: Tubulin beta chain

Chain F:  90% 6%

M1 C12 P32 P63 P82 F83 I86 G100 G106 G111 V122 C129 L132 H139 T145 M149 G150 T151 I154 I157 V171 E183 P184 I204 P222 T223 Y224 V231 D329 Q436 ASP ALA THR ALA ALA ASP GLN GLY ALA ASP GLN

GLY
GLU
PHE
GLU
GLU
GLU
GLY
GLU
ASP
GLU
ALA


- Molecule 2: Tubulin beta chain

Chain G:  90% 5%

M1 C12 P32 P63 P82 F83 I86 G106 G111 V122 C129 L132 H139 T145 M149 G150 T151 I154 I157 V171 E183 P184 I204 Y224 V231 D329 Q436 ASP ALA THR ALA ALA ASP GLN GLY ALA ASP GLU

GLU
GLU
GLY
GLU
GLU
ASP
GLU
ALA


- Molecule 2: Tubulin beta chain

Chain D:  90% 6%

M1 C12 P32 P63 P82 F83 I86 G100 G106 G111 V122 C129 L132 H139 T145 M149 G150 T151 I154 I157 V171 E183 P184 I204 P222 T223 Y224 V231 D329 Q436 ASP ALA THR ALA ALA ASP GLN GLY ALA ASP GLN

GLY
GLU
PHE
GLU
GLU
GLU
GLY
GLU
ASP
GLU
ALA

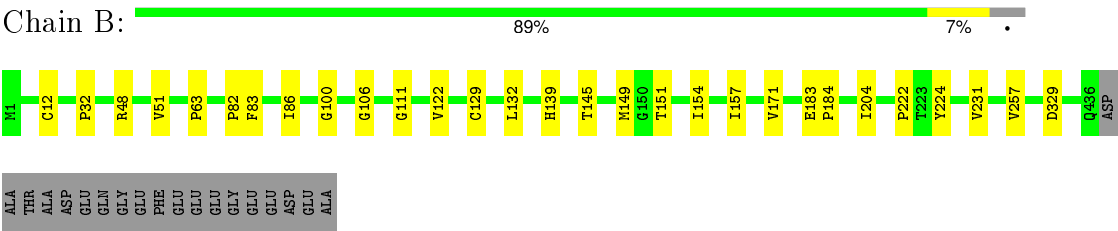
- Molecule 2: Tubulin beta chain

Chain I:  91% 5%

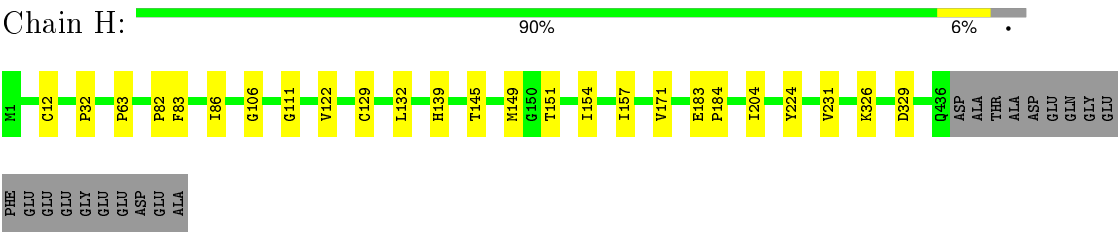
M1 C12 P32 P63 P82 F83 I86 G106 G111 C129 L132 H139 T145 M149 G150 T151 I154 V171 E183 P184 I204 Y224 V231 D329 Q436 ASP ALA THR ALA ASP GLU GLN GLY GLY PHE GLU GLU GLU GLU GLU

GLU
ASP
GLU
ALA

- Molecule 2: Tubulin beta chain



• Molecule 2: Tubulin beta chain



4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	CTFFIND4, each particle	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	27.6	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	27500	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, MG, G2P

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	A	0.44	0/3419	0.71	0/4643
1	C	0.45	0/3419	0.71	0/4643
1	E	0.44	0/3419	0.71	0/4643
1	J	0.45	0/3419	0.71	0/4643
1	K	0.45	0/3419	0.71	0/4643
1	L	0.45	0/3419	0.71	0/4643
2	B	0.45	0/3417	0.70	0/4631
2	D	0.45	0/3417	0.70	0/4631
2	F	0.45	0/3417	0.70	0/4631
2	G	0.45	0/3417	0.70	0/4631
2	H	0.45	0/3417	0.70	0/4631
2	I	0.45	0/3417	0.70	0/4631
All	All	0.45	0/41016	0.71	0/55644

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3342	0	3255	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3342	0	3255	13	0
1	E	3342	0	3255	11	0
1	J	3342	0	3255	8	0
1	K	3342	0	3255	12	0
1	L	3342	0	3255	10	0
2	B	3342	0	3219	20	0
2	D	3342	0	3219	16	0
2	F	3342	0	3219	16	0
2	G	3342	0	3219	14	0
2	H	3342	0	3219	16	0
2	I	3342	0	3219	13	0
3	A	32	0	12	0	0
3	C	32	0	12	0	0
3	E	32	0	12	0	0
3	J	32	0	12	0	0
3	K	32	0	12	0	0
3	L	32	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
5	B	32	0	14	0	0
5	D	32	0	14	0	0
5	F	32	0	14	0	0
5	G	32	0	14	0	0
5	H	32	0	14	0	0
5	I	32	0	14	0	0
All	All	40500	0	39000	139	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 139 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:151:THR:O	2:D:154:ILE:HG22	1.85	0.77
2:I:151:THR:O	2:I:154:ILE:HG22	1.85	0.77
2:H:151:THR:O	2:H:154:ILE:HG22	1.85	0.77
2:B:151:THR:O	2:B:154:ILE:HG22	1.85	0.76
2:F:151:THR:O	2:F:154:ILE:HG22	1.85	0.76

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	424/451 (94%)	410 (97%)	13 (3%)	1 (0%)	52	88
1	C	424/451 (94%)	410 (97%)	13 (3%)	1 (0%)	52	88
1	E	424/451 (94%)	410 (97%)	13 (3%)	1 (0%)	52	88
1	J	424/451 (94%)	410 (97%)	13 (3%)	1 (0%)	52	88
1	K	424/451 (94%)	410 (97%)	13 (3%)	1 (0%)	52	88
1	L	424/451 (94%)	410 (97%)	13 (3%)	1 (0%)	52	88
2	B	424/445 (95%)	411 (97%)	13 (3%)	0	100	100
2	D	424/445 (95%)	411 (97%)	13 (3%)	0	100	100
2	F	424/445 (95%)	411 (97%)	13 (3%)	0	100	100
2	G	424/445 (95%)	411 (97%)	13 (3%)	0	100	100
2	H	424/445 (95%)	411 (97%)	13 (3%)	0	100	100
2	I	424/445 (95%)	411 (97%)	13 (3%)	0	100	100
All	All	5088/5376 (95%)	4926 (97%)	156 (3%)	6 (0%)	59	90

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	2	ARG

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Mol	Chain	Res	Type
1	J	2	ARG
1	C	2	ARG
1	L	2	ARG
1	A	2	ARG

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	357/379 (94%)	353 (99%)	4 (1%)	80	92
1	C	357/379 (94%)	353 (99%)	4 (1%)	80	92
1	E	357/379 (94%)	353 (99%)	4 (1%)	80	92
1	J	357/379 (94%)	353 (99%)	4 (1%)	80	92
1	K	357/379 (94%)	353 (99%)	4 (1%)	80	92
1	L	357/379 (94%)	353 (99%)	4 (1%)	80	92
2	B	365/381 (96%)	363 (100%)	2 (0%)	92	97
2	D	365/381 (96%)	363 (100%)	2 (0%)	92	97
2	F	365/381 (96%)	363 (100%)	2 (0%)	92	97
2	G	365/381 (96%)	363 (100%)	2 (0%)	92	97
2	H	365/381 (96%)	363 (100%)	2 (0%)	92	97
2	I	365/381 (96%)	363 (100%)	2 (0%)	92	97
All	All	4332/4560 (95%)	4296 (99%)	36 (1%)	87	95

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	139	HIS
1	L	225	THR
1	K	437	VAL
1	L	27	GLU
1	L	437	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	136	GLN
1	L	228	ASN
1	A	329	ASN
1	C	300	ASN
1	C	329	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 12 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GTP	A	501	4	26,34,34	1.10	2 (7%)	29,54,54	1.96	5 (17%)
5	G2P	B	501	4	29,34,34	1.92	8 (27%)	32,54,54	2.35	14 (43%)
3	GTP	C	501	4	26,34,34	1.09	2 (7%)	29,54,54	1.91	5 (17%)
5	G2P	D	501	4	29,34,34	1.99	10 (34%)	32,54,54	2.33	12 (37%)
3	GTP	E	501	4	26,34,34	1.11	2 (7%)	29,54,54	1.96	5 (17%)
5	G2P	F	501	4	29,34,34	2.00	8 (27%)	32,54,54	2.44	14 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	G2P	G	501	4	29,34,34	2.00	9 (31%)	32,54,54	2.47	14 (43%)
5	G2P	H	501	4	29,34,34	1.95	9 (31%)	32,54,54	2.41	13 (40%)
5	G2P	I	501	4	29,34,34	1.94	8 (27%)	32,54,54	2.36	13 (40%)
3	GTP	J	501	4	26,34,34	1.06	2 (7%)	29,54,54	1.85	5 (17%)
3	GTP	K	501	4	26,34,34	1.04	2 (7%)	29,54,54	1.85	5 (17%)
3	GTP	L	501	4	26,34,34	1.05	2 (7%)	29,54,54	1.81	5 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GTP	A	501	4	-	0/18/38/38	0/3/3/3
5	G2P	B	501	4	-	0/15/38/38	0/3/3/3
3	GTP	C	501	4	-	0/18/38/38	0/3/3/3
5	G2P	D	501	4	-	0/15/38/38	0/3/3/3
3	GTP	E	501	4	-	0/18/38/38	0/3/3/3
5	G2P	F	501	4	-	0/15/38/38	0/3/3/3
5	G2P	G	501	4	-	0/15/38/38	0/3/3/3
5	G2P	H	501	4	-	0/15/38/38	0/3/3/3
5	G2P	I	501	4	-	0/15/38/38	0/3/3/3
3	GTP	J	501	4	-	0/18/38/38	0/3/3/3
3	GTP	K	501	4	-	0/18/38/38	0/3/3/3
3	GTP	L	501	4	-	0/18/38/38	0/3/3/3

The worst 5 of 64 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	501	G2P	PB-O1B	-3.56	1.47	1.56
5	D	501	G2P	PB-O1B	-3.55	1.47	1.56
5	B	501	G2P	PB-O1B	-3.53	1.47	1.56
5	H	501	G2P	PB-O1B	-3.50	1.48	1.56
5	I	501	G2P	PB-O1B	-3.48	1.48	1.56

The worst 5 of 110 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	GTP	C1'-N9-C4	-4.56	121.72	126.81
5	G	501	G2P	O4'-C4'-C3'	-4.54	95.95	105.16
3	E	501	GTP	C1'-N9-C4	-4.47	121.82	126.81

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
5	G	501	G2P	C5-C6-N1	-4.43	117.73	123.52
5	H	501	G2P	C5-C6-N1	-4.41	117.75	123.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.